Numerical Homogenization of Trabecular Bone Specimens using Composite Finite Elements

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University of Bonn

Joint work with: Martin Rumpf (INS Bonn)
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Bonn, 2010–06–22

Preview: Effective Elasticity Tensors

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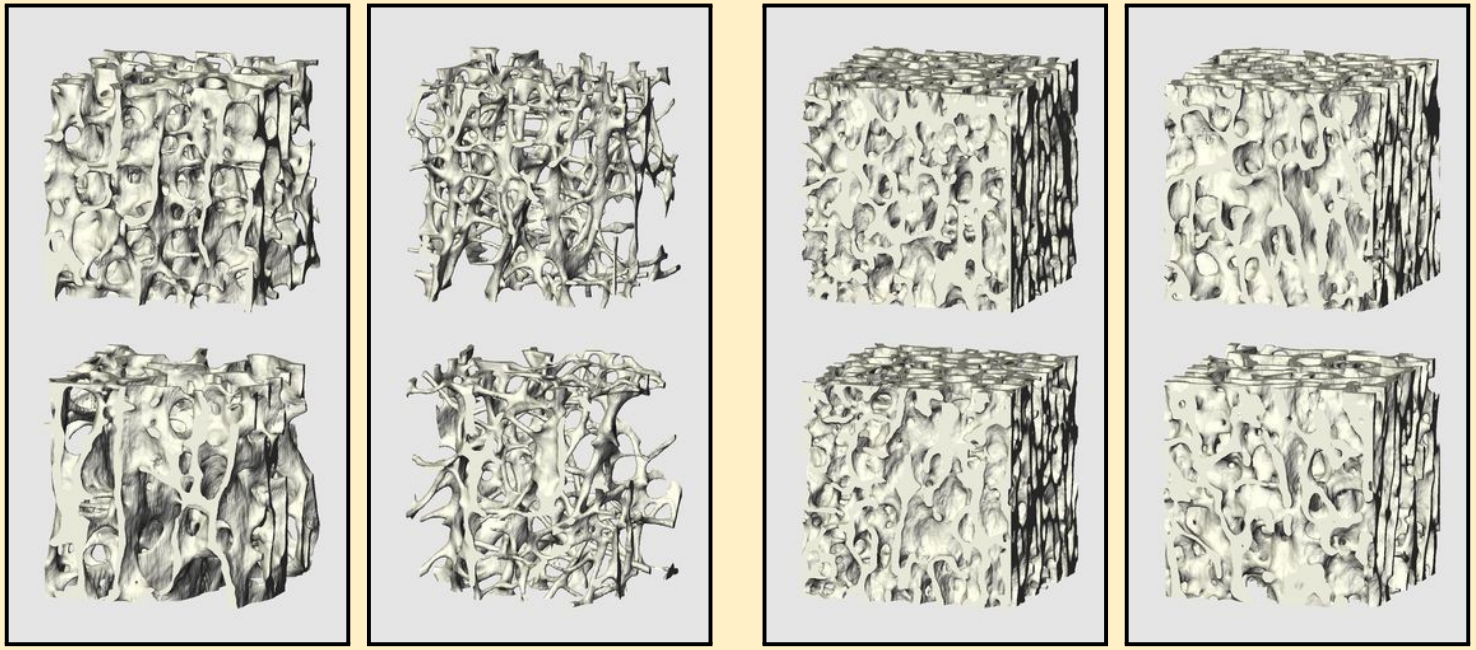
Goal: two-scale simulation of vertebrae

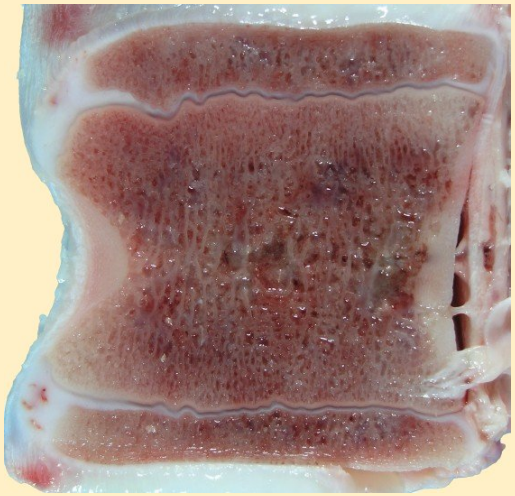
human ♂ young | human ♀ osteoporotic | porcine | bovine



Method: determine effective elasticity parameters of statistically periodic trabecular microstructures

Specimen Acquisition

- Harvested vertebrae from spines of
  - young ♂ human
  - osteoporotic ♀ human
  - pig
  - cow



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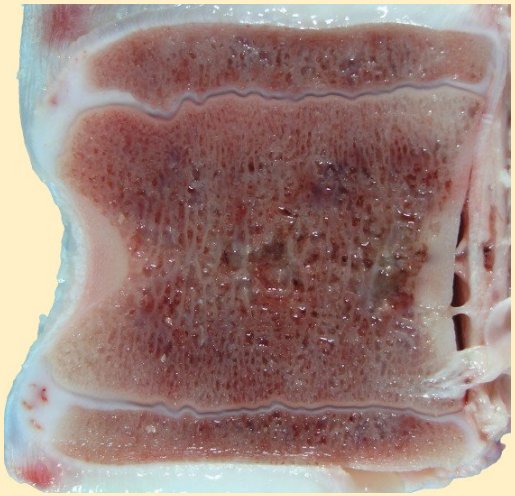
- μCT scans at 40 μm
- cubic specimens of edge length 5.16 mm



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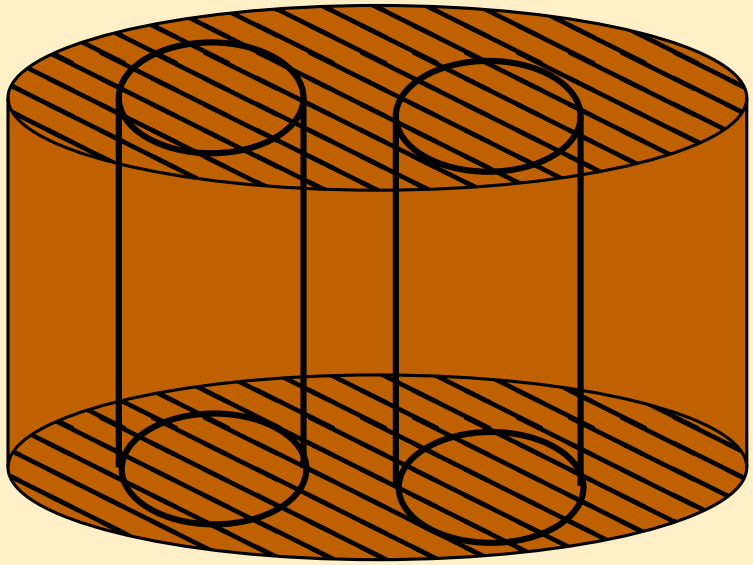

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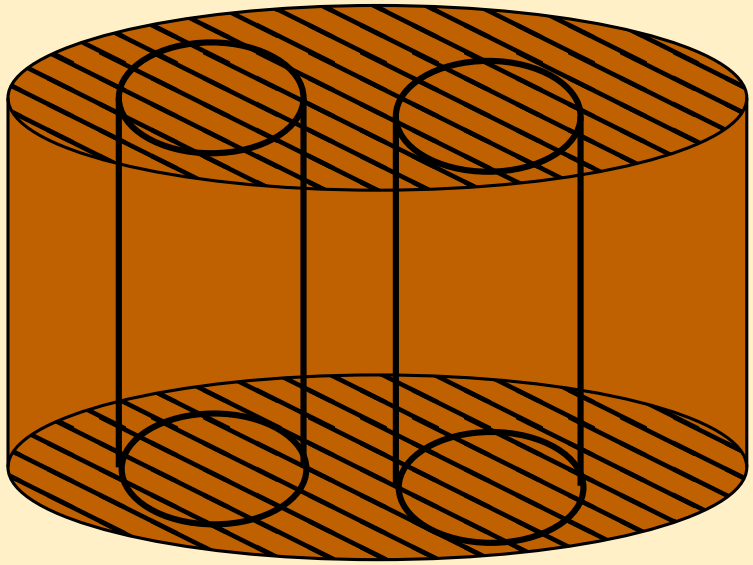

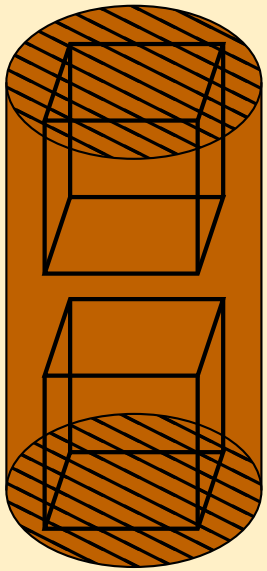

Linearized Elasticity Model

Microscopic material parameters (isotropic):

- Young's modulus (stiffness) $E = 13$ GPa
- Poisson's ratio (bulging ratio) $\nu = 0.32$

[Wolfram, Wilke, Zysset Bone 46:348]

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[Wolfram, Wilke, Zysset Bone 46:348]

Displacement $u : \Omega^{\#} \to \mathbb{R}^3$

Elasticity tensor C couples

- strain $\epsilon(u) = \frac{1}{2}\left[\nabla u + (\nabla u)^T\right]$
- and stress σ via $\sigma = C\epsilon(u)$

Numerical Homogenization (Exactly Periodic Case)

Determine effective elasticity tensor by imposing different unit strains and computing stress response.

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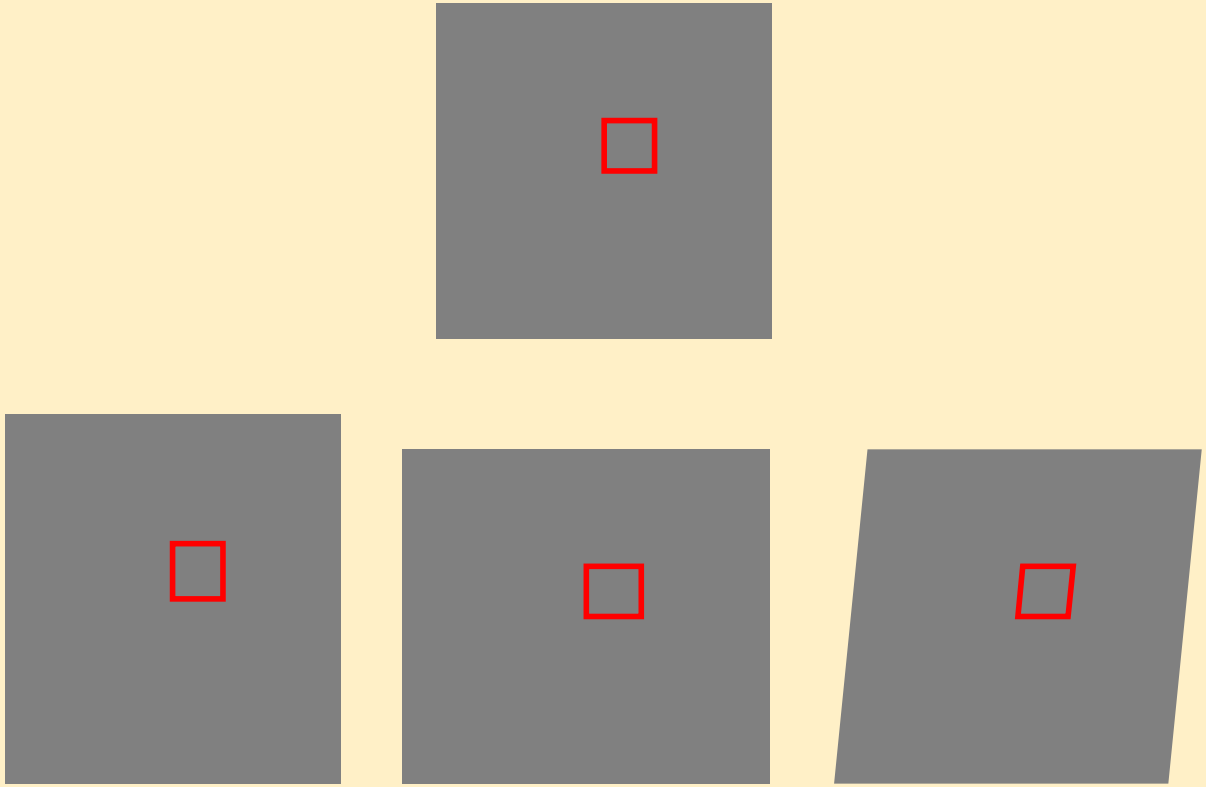

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- macroscopic unit strain $\bar{u}$ and
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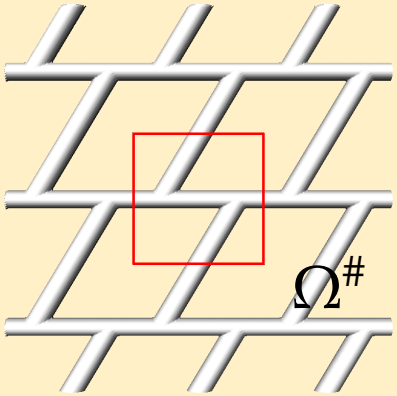

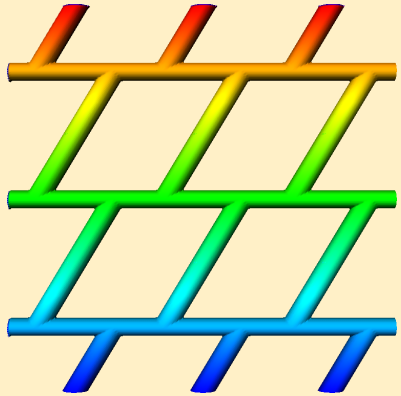

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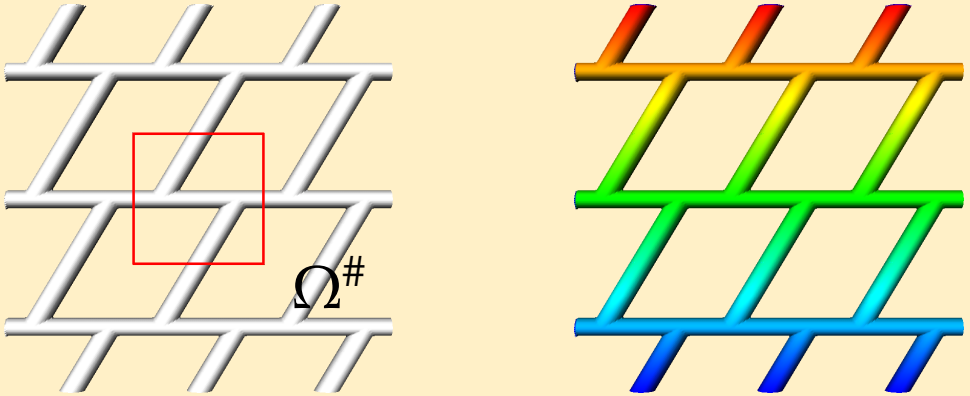

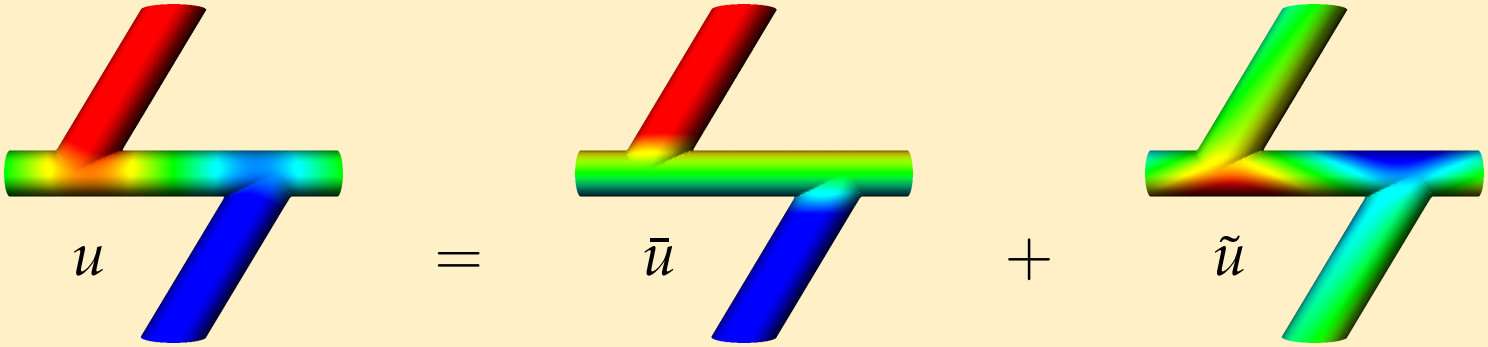

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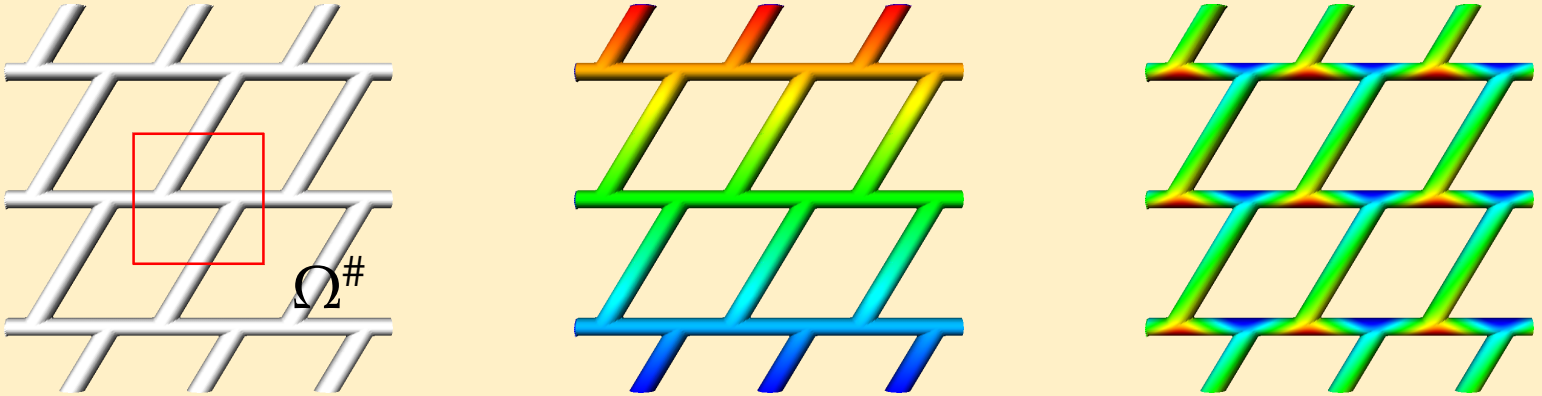

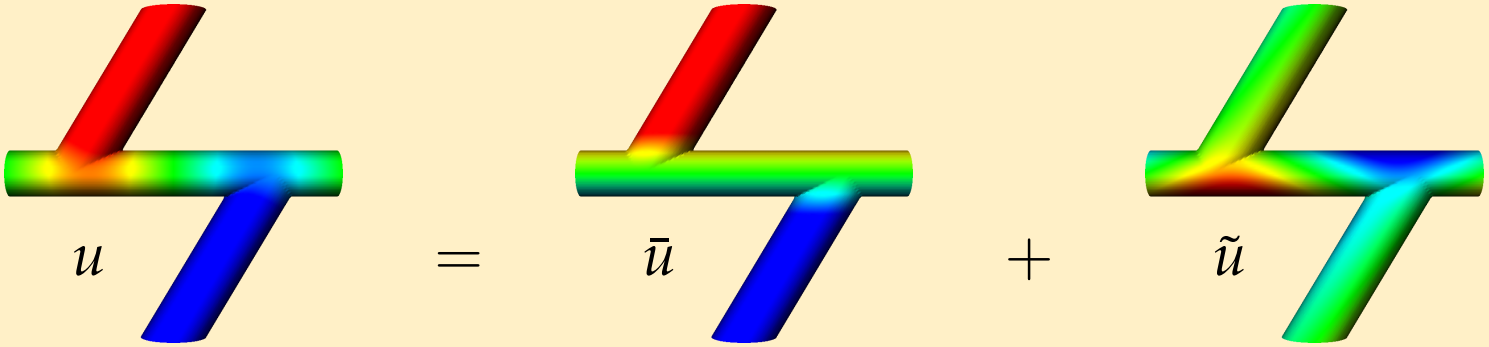

z displacement

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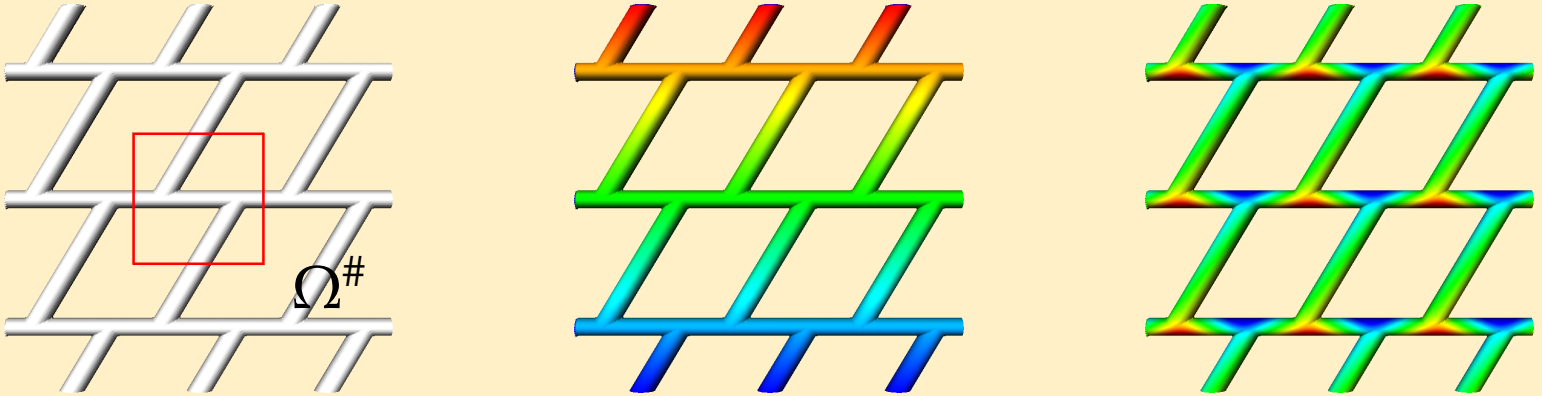

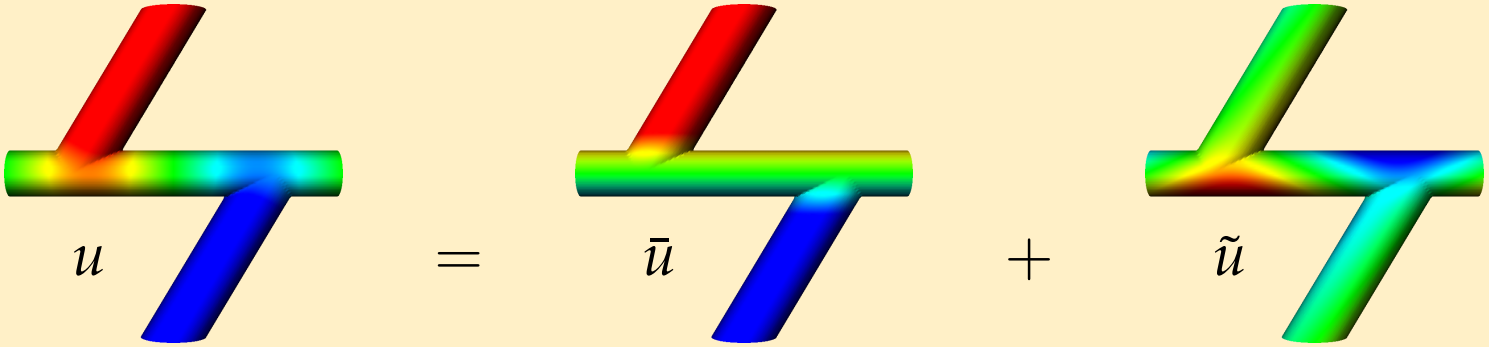

Let's make this more precise ...

 z displacement

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Decompose physical displacement $u = \bar{u} + \tilde{u}$ in

- macroscopic strain $\bar{u}$ (given) and
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Elasticity equation:

$$\begin{aligned} & -\operatorname{div} C\epsilon(u) = 0 \\ \Rightarrow \quad & -\operatorname{div} C\epsilon(\tilde{u}) = \operatorname{div} C\epsilon(\bar{u}) \end{aligned}$$

To ensure uniqueness of the decomposition, require $\fint_{\Omega^\#} \tilde{u} = 0$.

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$$\bar{C}_{..ij} = \bar{\sigma}^{ij} = \fint_{\Omega^\#} C\Big[\underbrace{\epsilon(\bar{u}^{ij})}_{e_{ij}} + \epsilon(\tilde{u}^{ij})\Big]$$

Numerical Homogenization (Statistically Periodic Case)

In case of non-periodic microstructures, need statistically representative fundamental cell of at least 5 inter-trabecular distances [Harrigan et al, JBiomech 21:269].

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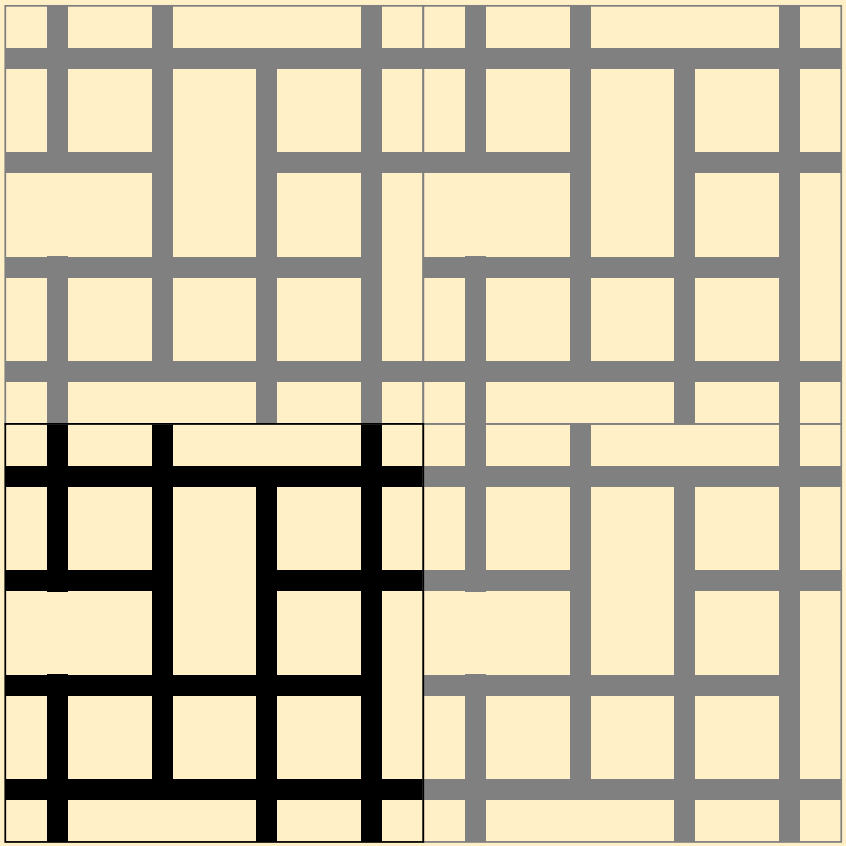

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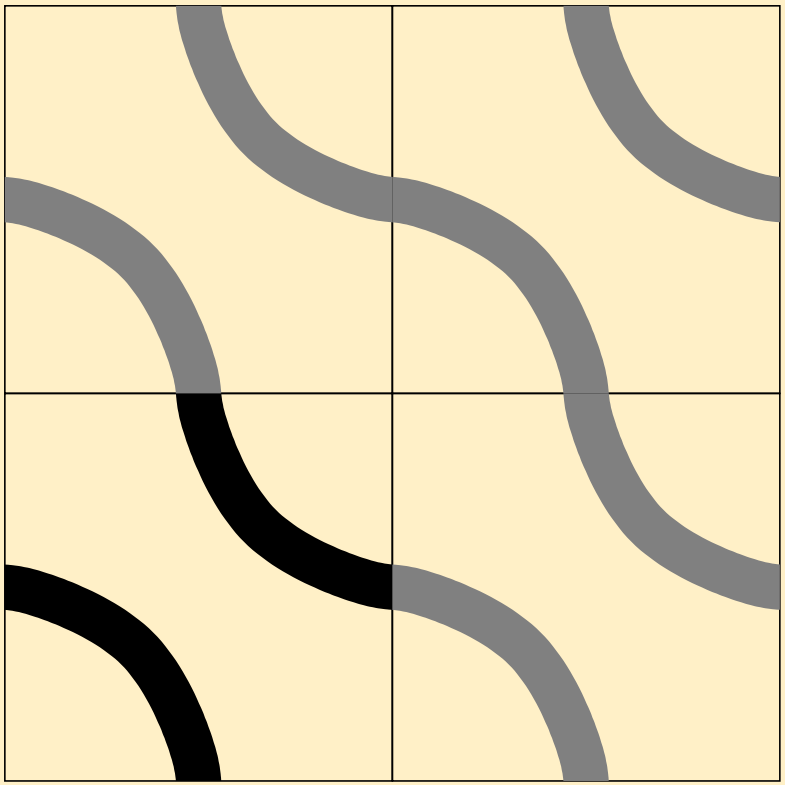

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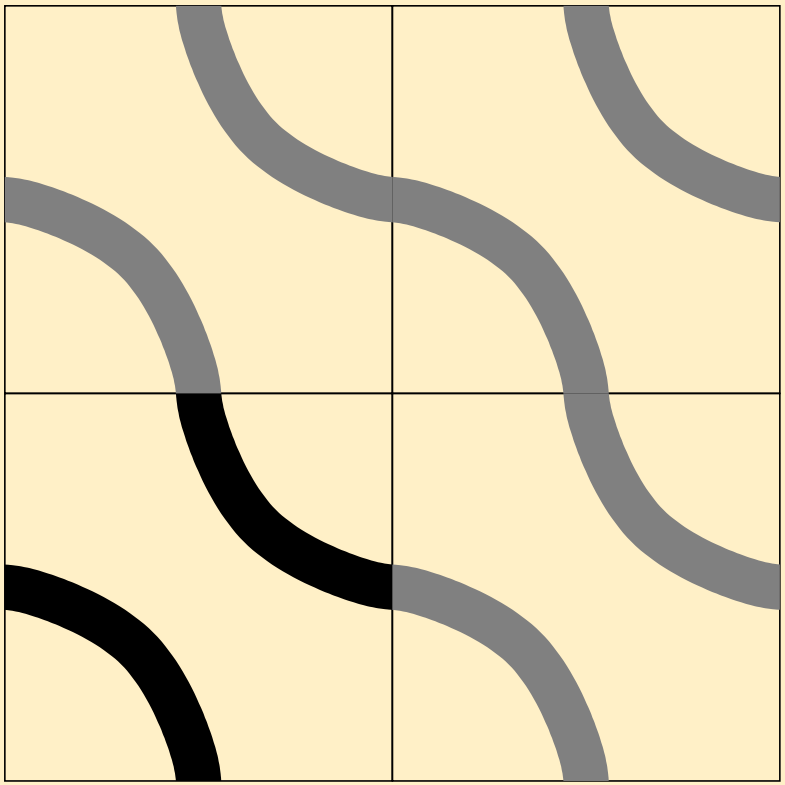
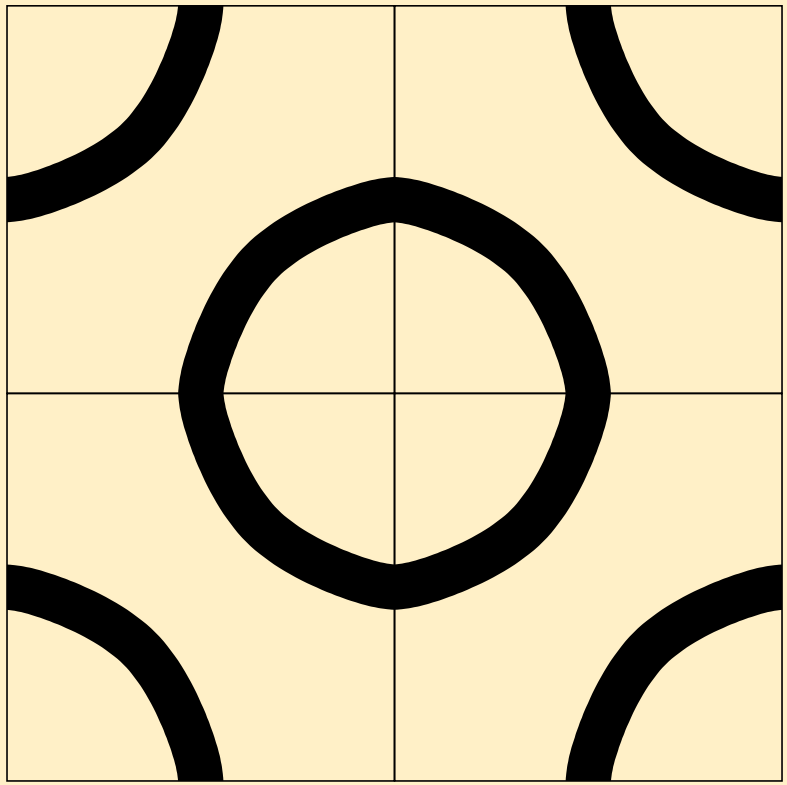
Could make structure periodic by mirroring, but that is a bad idea.





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For $\bar{u}^{ij} = e_{ij} := \frac{1}{2}(e_i \otimes e_j + e_j \otimes e_i)$ (as before), consider

$$\begin{aligned} -\operatorname{div}\left(C\epsilon(u^{ij})\right) &= 0 \quad && \text{in } \Omega^{\#} \\ u^{ij} &= \bar{u}^{ij} && \text{on } \partial^{\square}\Omega^{\#} \end{aligned}$$

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The average stress is then evaluated as

$$\left[\bar{C}_{ij\cdot\cdot} = \right]\bar{\sigma}^{ij} = \fint_{\Omega^{\#}_{\beta}} C\epsilon[u^{ij}]\,.$$

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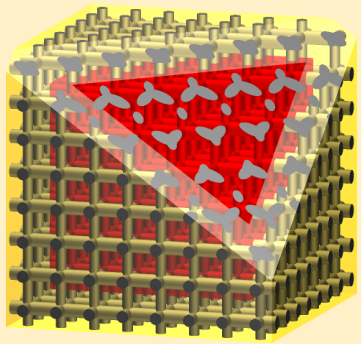
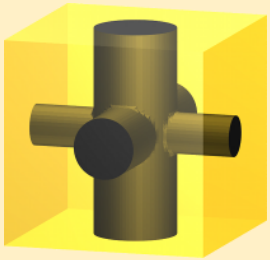
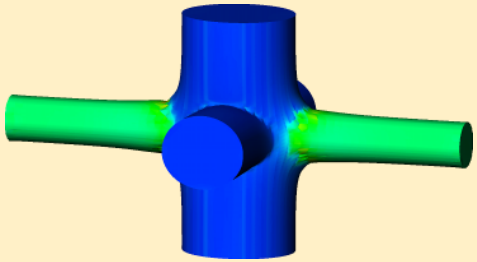
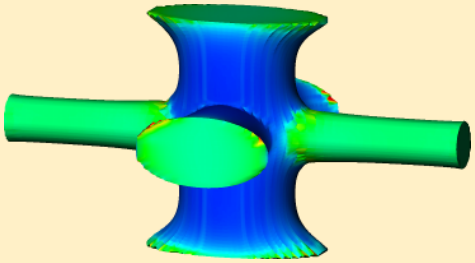


$\Omega^{\#}_{\beta} = \{x \in \Omega^{\#} \mid \operatorname{dist}(x, \partial^{\square}\Omega^{\#} > \beta\}$. Why?

Numerical Homogenization (Statistically Periodic Case)

Problem: artificial stiffening near the boundary by enforcing displacement boundary conditions (right)

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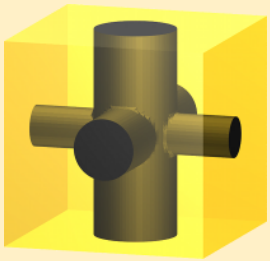
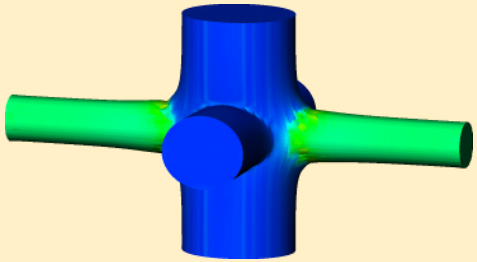
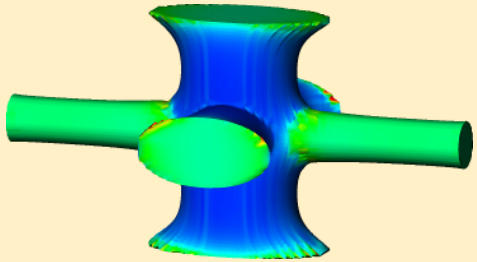
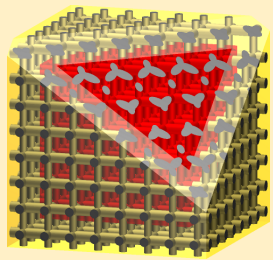




Solution: ignore boundary layer and
evaluate stress only in interior $\Omega_\beta^\#$ (typically $\beta = 0.125$)

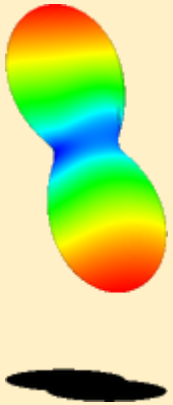
cf. [Ün, Bevill, Keaveny J Biomech 39:1955]



Note that $\Omega_\beta^\#$ still needs to be representative.

Tensor Rotation and Visualization

Tensors are visualized as deformed (encoding uniaxial stiffness) and colored (encodes bulk modulus) spheres.



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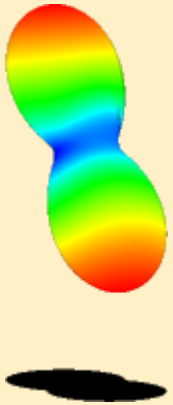

Orthotropy? Axes of orthotropy?

Determine rotation matrix $Q \in \mathrm{SO}(3)$ (with angle bound) minimizing orthotropy violation

$$F_{\bar{C}}(Q) = \frac{\|R_a[\bar{C}^Q]\|_F^2}{\|R_b[\bar{C}^Q]\|_F^2} \quad \text{where } \bar{C}^Q := Q_{mi}Q_{nj}Q_{pk}Q_{ql}\bar{C}_{ijkl}$$

$$\bar{C} = \begin{bmatrix} 0.3926 & 0.1726 & 0.1771 & -0.0013 & -0.0088 & -0.0304 \\ 0.1726 & 0.3678 & 0.1804 & -0.0010 & 0.0073 & -0.0108 \\ 0.1771 & 0.1804 & 1.0276 & -0.0111 & 0.0218 & -0.0032 \\ -0.0013 & -0.0010 & -0.0111 & 0.1668 & -0.0305 & 0.0064 \\ -0.0088 & 0.0073 & 0.0218 & -0.0305 & 0.1718 & -0.0022 \\ -0.0304 & -0.0108 & -0.0032 & 0.0064 & -0.0022 & 0.0907 \end{bmatrix}$$

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$$\bar{C}^Q = \begin{bmatrix} 0.4090 & 0.1856 & 0.1809 & -0.0039 & -0.0018 & 0.0164 \\ 0.1856 & 0.3260 & 0.1749 & 0.0004 & -0.0051 & -0.0045 \\ 0.1809 & 0.1749 & 1.0302 & 0.0018 & 0.0016 & -0.0027 \\ -0.0039 & 0.0004 & 0.0018 & 0.1380 & 0.0005 & -0.0073 \\ -0.0018 & -0.0051 & 0.0016 & 0.0005 & 0.1988 & -0.0059 \\ 0.0164 & -0.0045 & -0.0027 & -0.0073 & -0.0059 & 0.1038 \end{bmatrix}$$

Discretization

Discretization by Composite Finite Elements

[Hackbusch, Sauter Numer Math 75:447; Comp Vis Sci 1:15]

[Liehr/Preusser/Rumpf/Sauter/S. Comp Vis Sci 12:171]

Results for Individual Specimens

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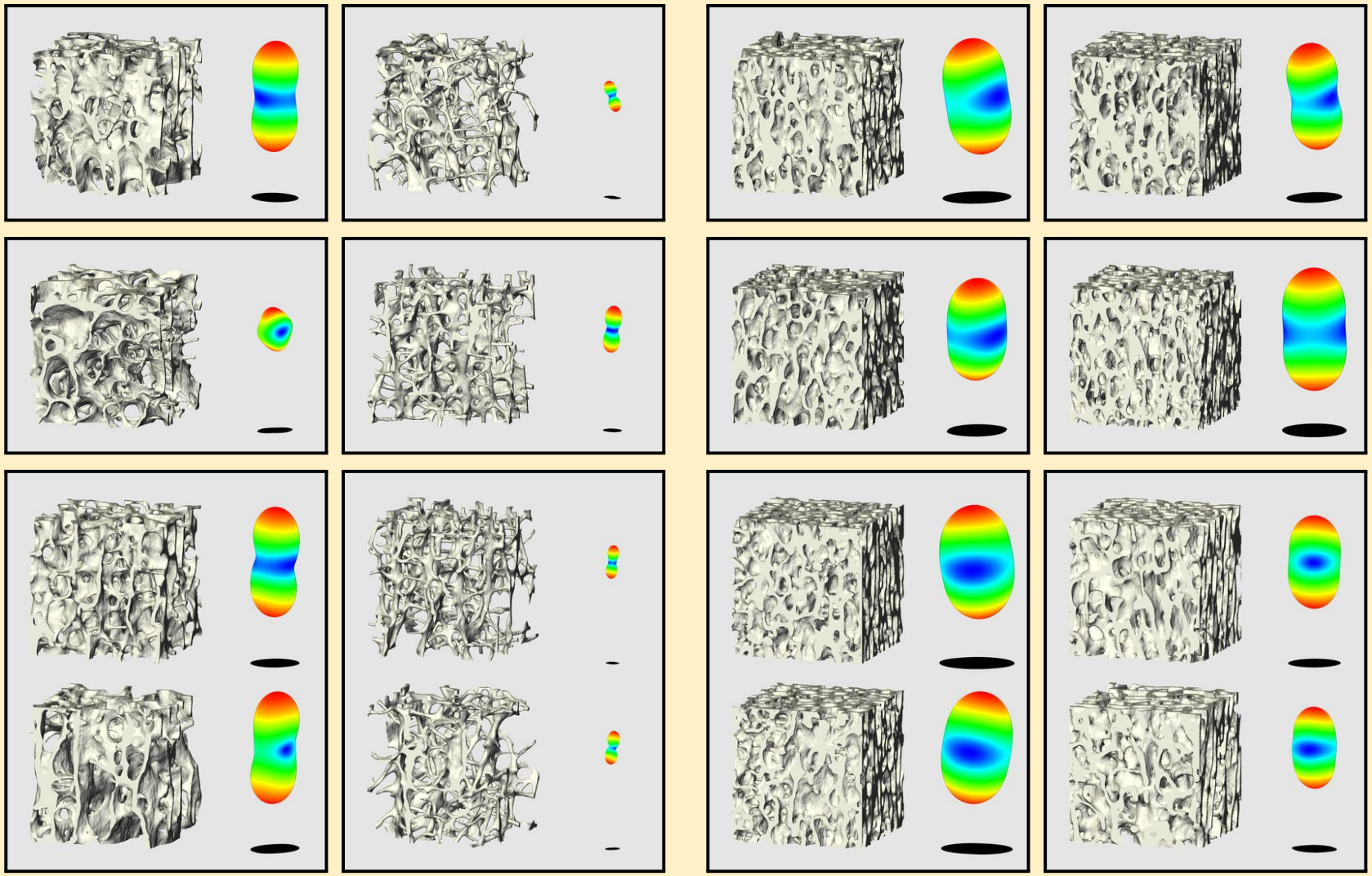

human tensors scaled by 4

Differences Between Species (Averages)

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species	human-y	human-o	porcine	bovine
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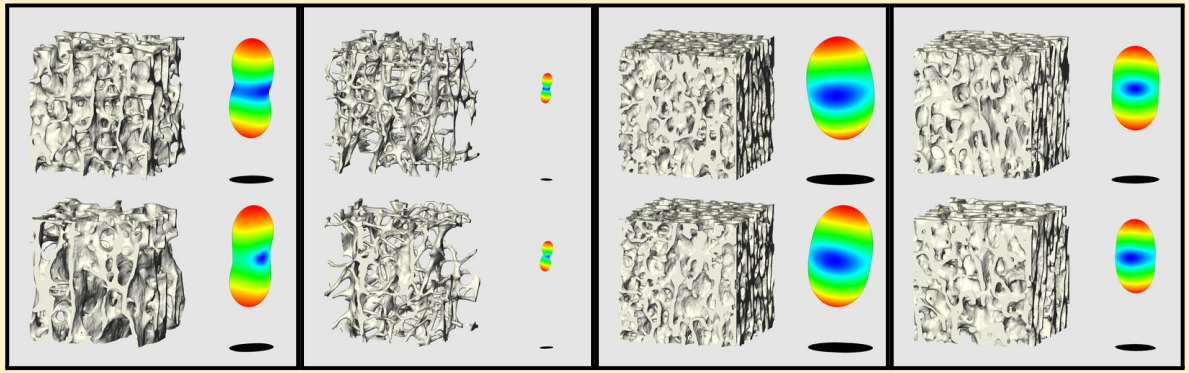
volume fraction	0.141	0.081	0.370	0.330
E_{zz} in GPa	0.812	0.383	3.456	3.203
$\frac{E_{xx}+E_{yy}}{2}$ in GPa	0.334	0.130	1.831	1.263
anisotropy $\frac{2E_{zz}}{E_{xx}+E_{yy}}$	2.550	4.054	1.891	2.635

examples



scaled by 4

z: aligned craniocaudal direction; x, y: aligned transverse directions

Differences Between Species (Averages)

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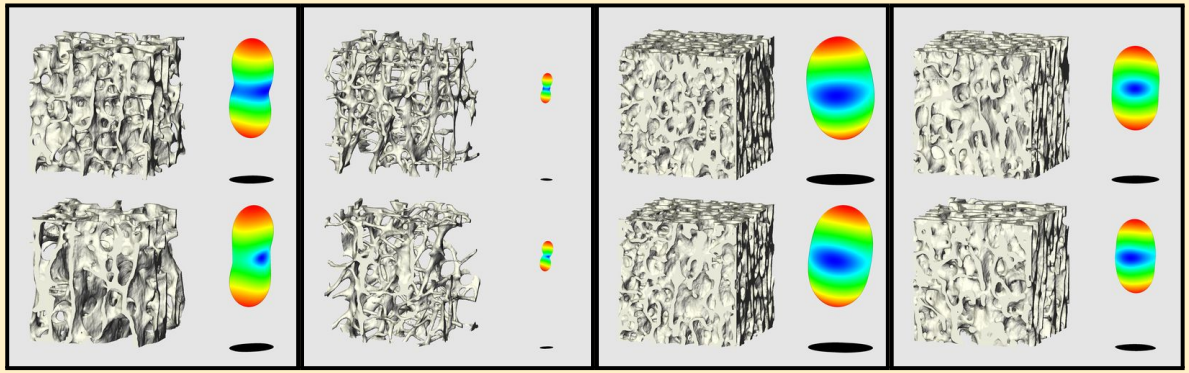

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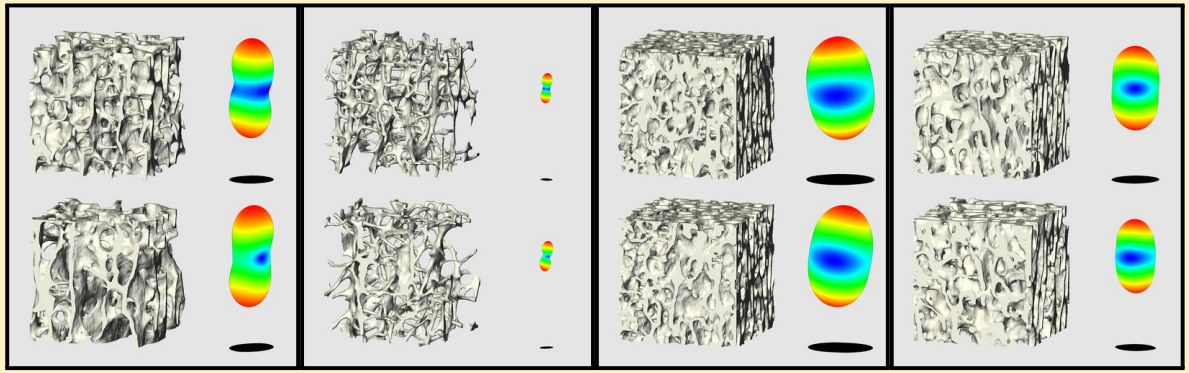

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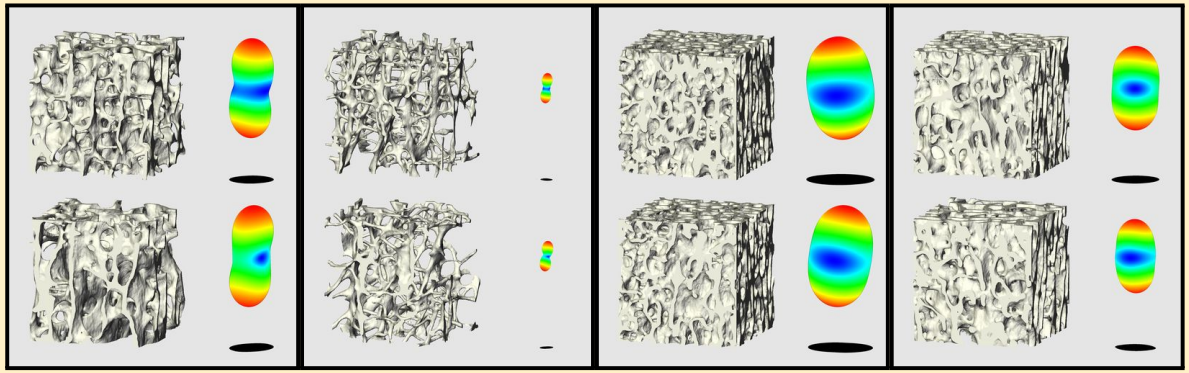

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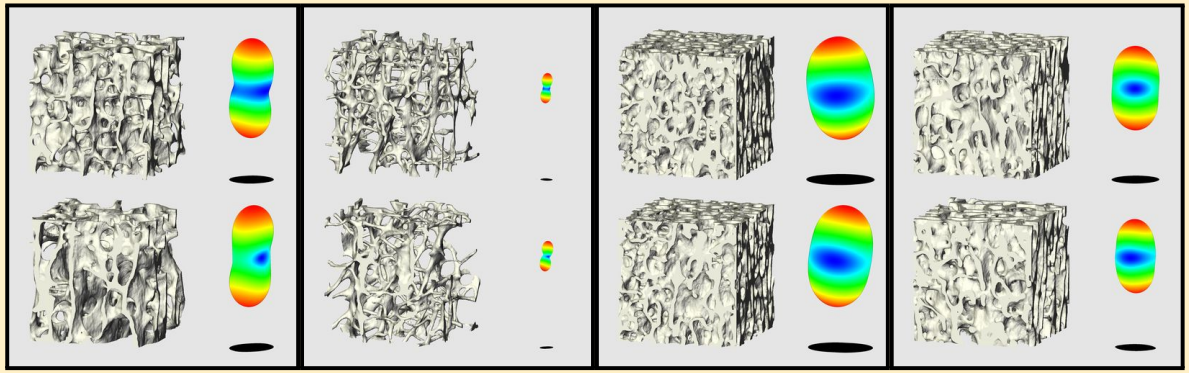

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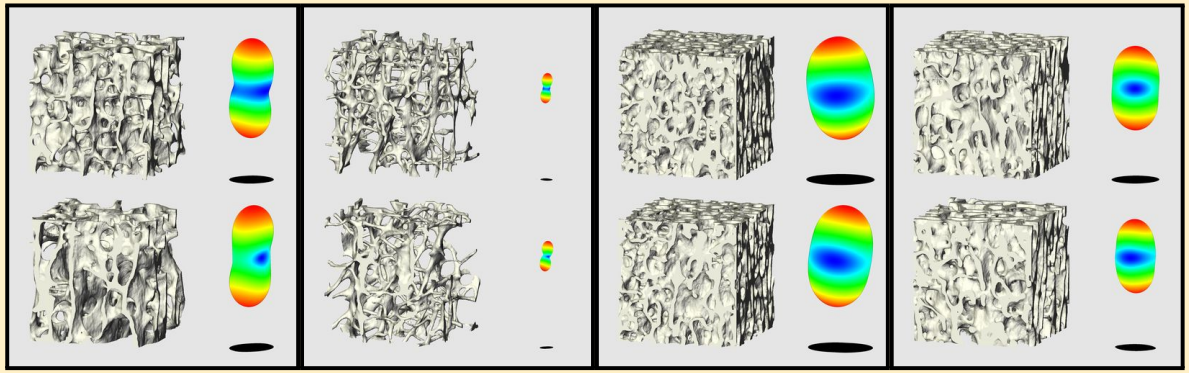

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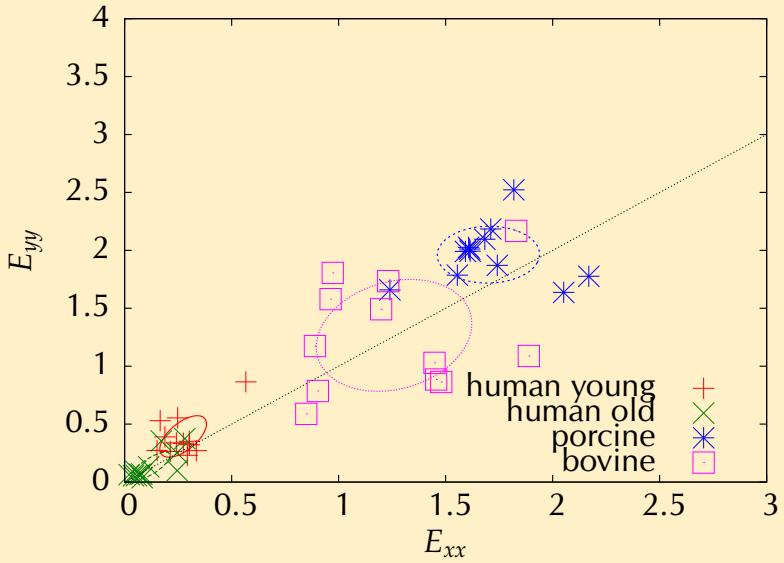
Differences Between Species (2)

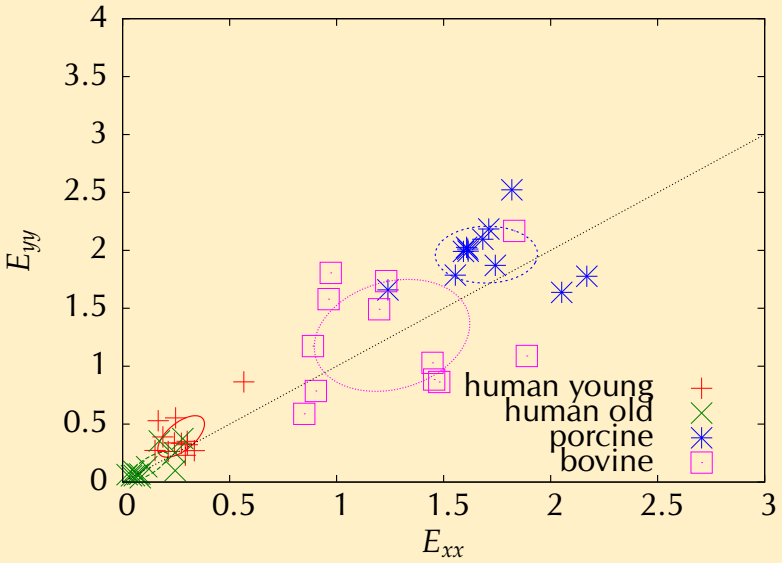


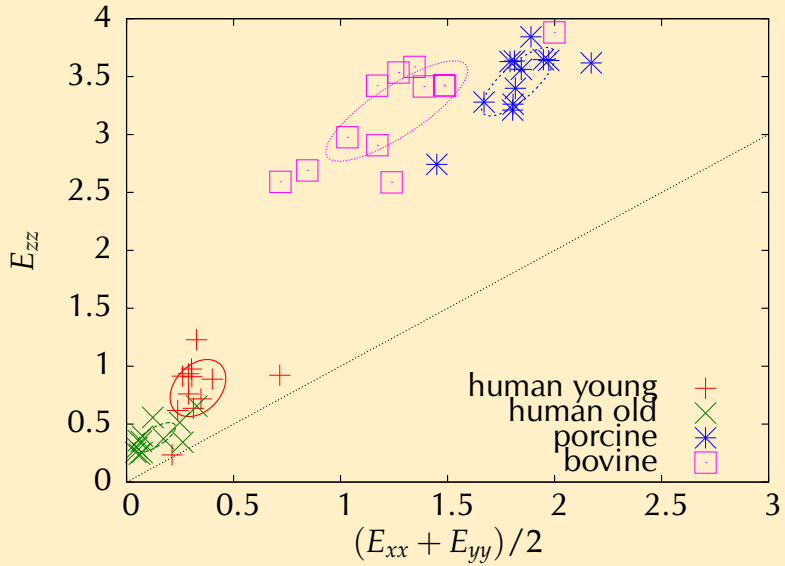
(ellipses: 1 standard deviation obtained by PCA)

Interpretation:

- transverse isotropy?

Differences Between Species (2)





(ellipses: 1 standard deviation obtained by PCA)

Interpretation:

- transverse isotropy?
- anisotropy: craniocaudal/average transverse
- distinct clusters

Differences for a Single Vertebra

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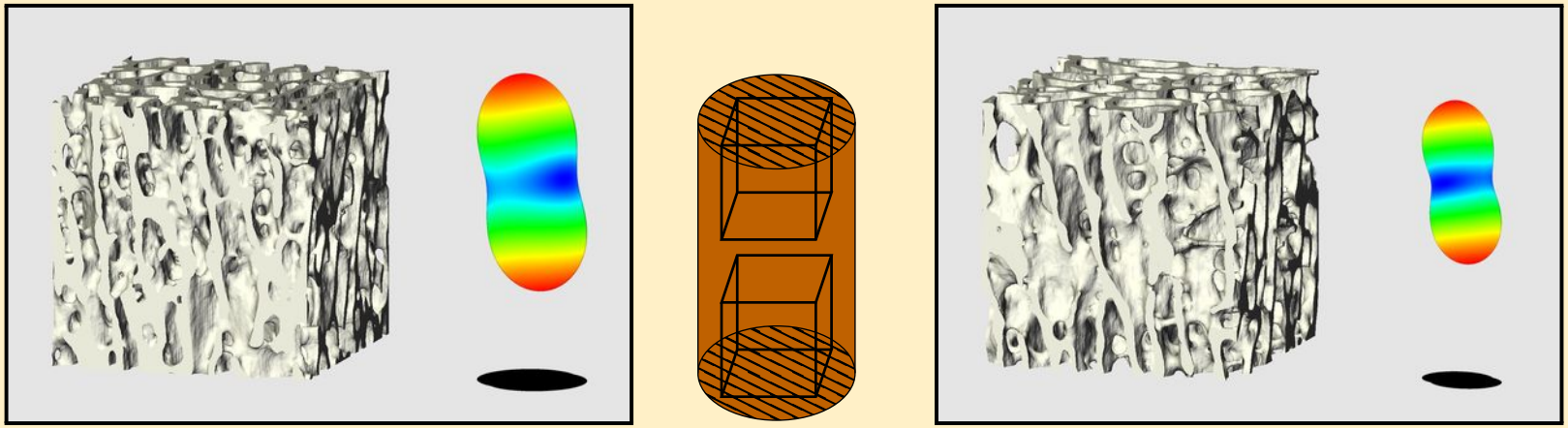
Need full two-scale model, cannot consider spongious interior as homogeneous material.



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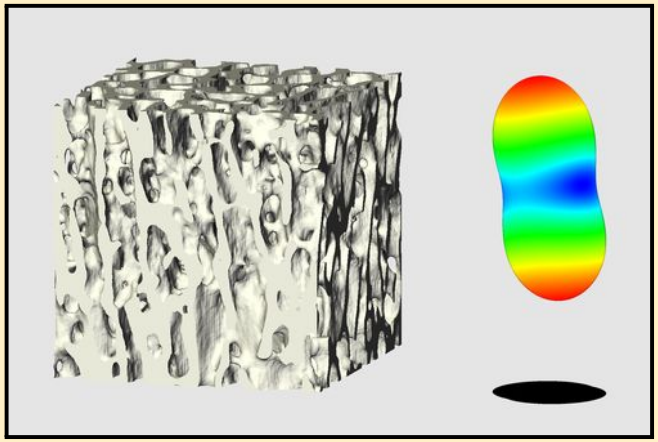

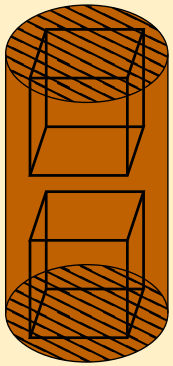

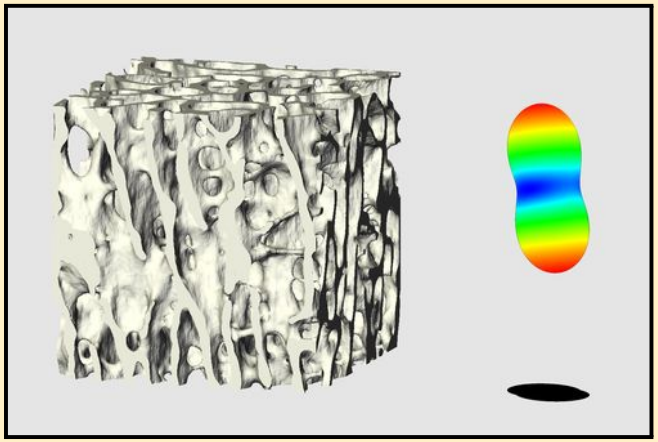

roll $= -7.52°$, pitch $= 9.44°$,
yaw $= -18.22°$

$E_{xx} = 1.199$, $E_{yy} = 1.492$,
$E_{zz} = 3.584$ GPa

roll $= -12.27°$, pitch $= 10.75°$,
yaw $= -26.27°$

$E_{xx} = 0.903$, $E_{yy} = 0.786$,
$E_{zz} = 2.690$ GPa

Summary

- homogenization method for statistically periodic trabecular microstructures
- some understanding of macroscopic properties of animal and human vertebral trabecular bone

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- homogenization method for statistically periodic trabecular microstructures
- some understanding of macroscopic properties of animal and human vertebral trabecular bone
- limitations:
  - simple linear elasticity model (no plasticity or cracks)
  - uncertain material parameters (human vs. animal)
  - only 12 specimens per species
  - dorsoventral and dextrosinistral axes unknown
  - validation of Composite FE pending

References

- F. Liehr, T. Preusser, M. Rumpf, S. Sauter, and L. O. Schwen: *Composite Finite Elements for 3D Image Based Computing*, Computing and Visualization in Science 12(4), pp. 171–188, 2009
- L. O. Schwen, U. Wolfram, H.-J. Wilke, and M. Rumpf, *Determining effective elasticity parameters of microstructured materials*, Proceedings of the 15th Workshop on the Finite Element Method in Biomedical Engineering, Biomechanics and Related Fields, University of Ulm, July 2008, pp. 41–62
- T. Preusser, M. Rumpf, S. Sauter, and L. O. Schwen, *3D composite finite elements for elliptic boundary value problems with discontinuous coefficients*, submitted to SIAM Journal on Scientific Computing

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